

链霉菌 *Streptomyces* sp. neau-D50 中的一个新天然产物

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补充数据

A New Natural Product from *Streptomyces* sp. neau-D50

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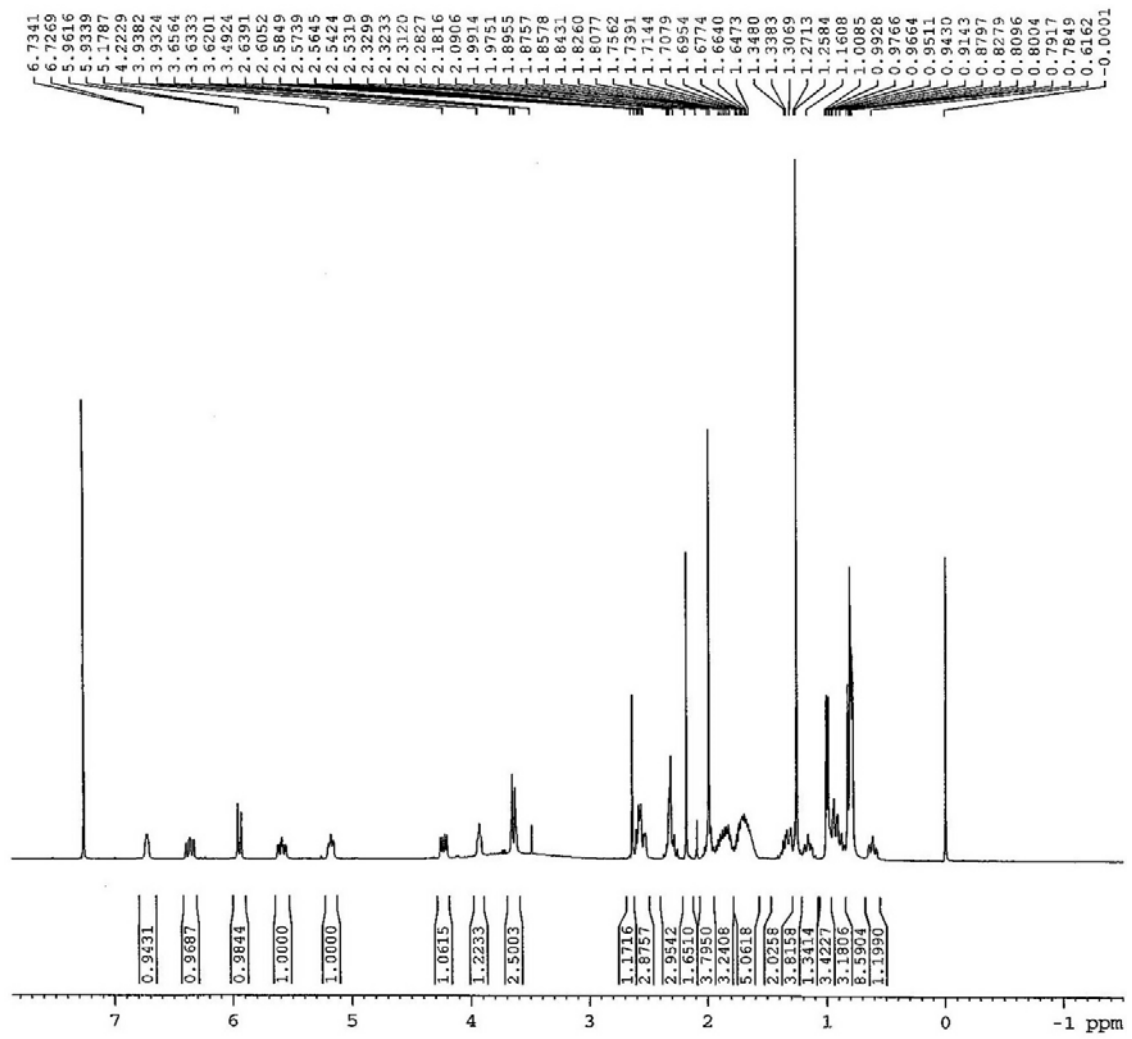
Zhejiang Hisun Pharmaceutical Co., Ltd., Taizhou, Zhejiang 318000, China

Supporting data

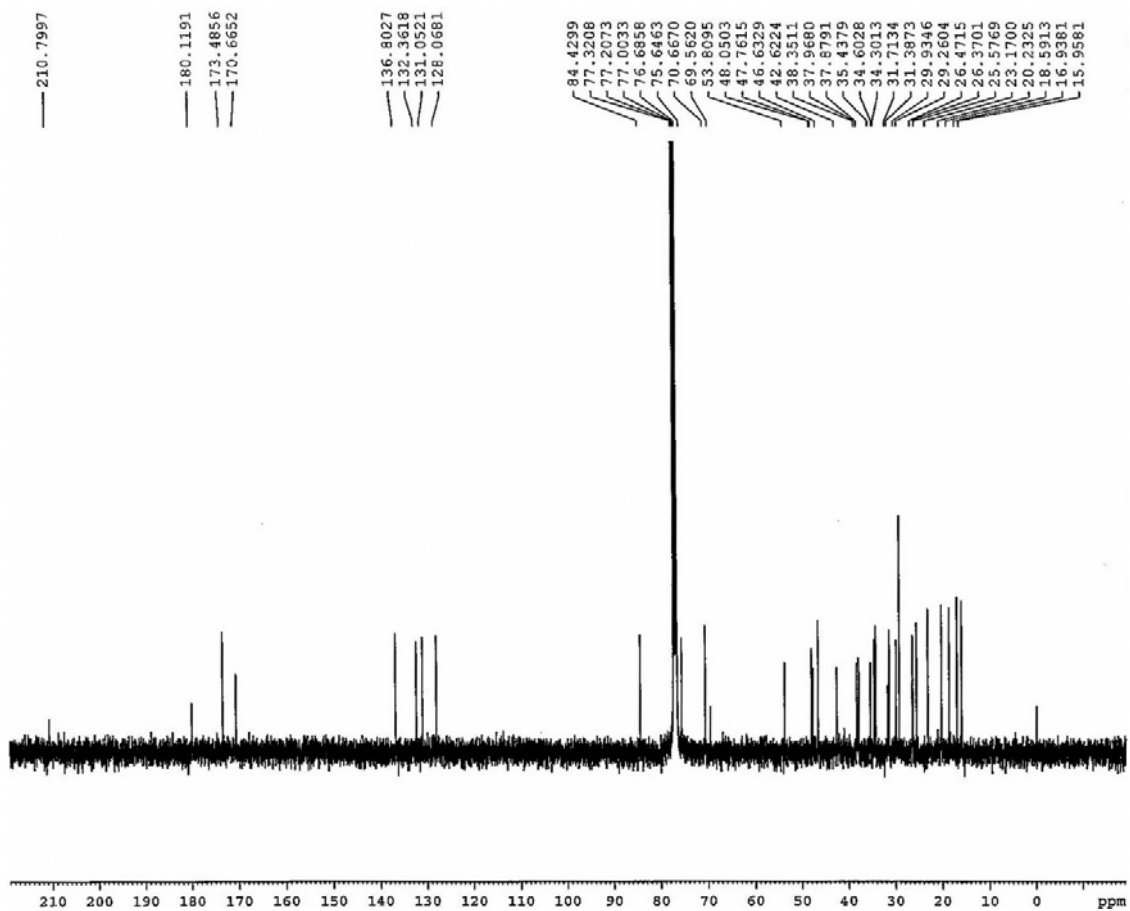
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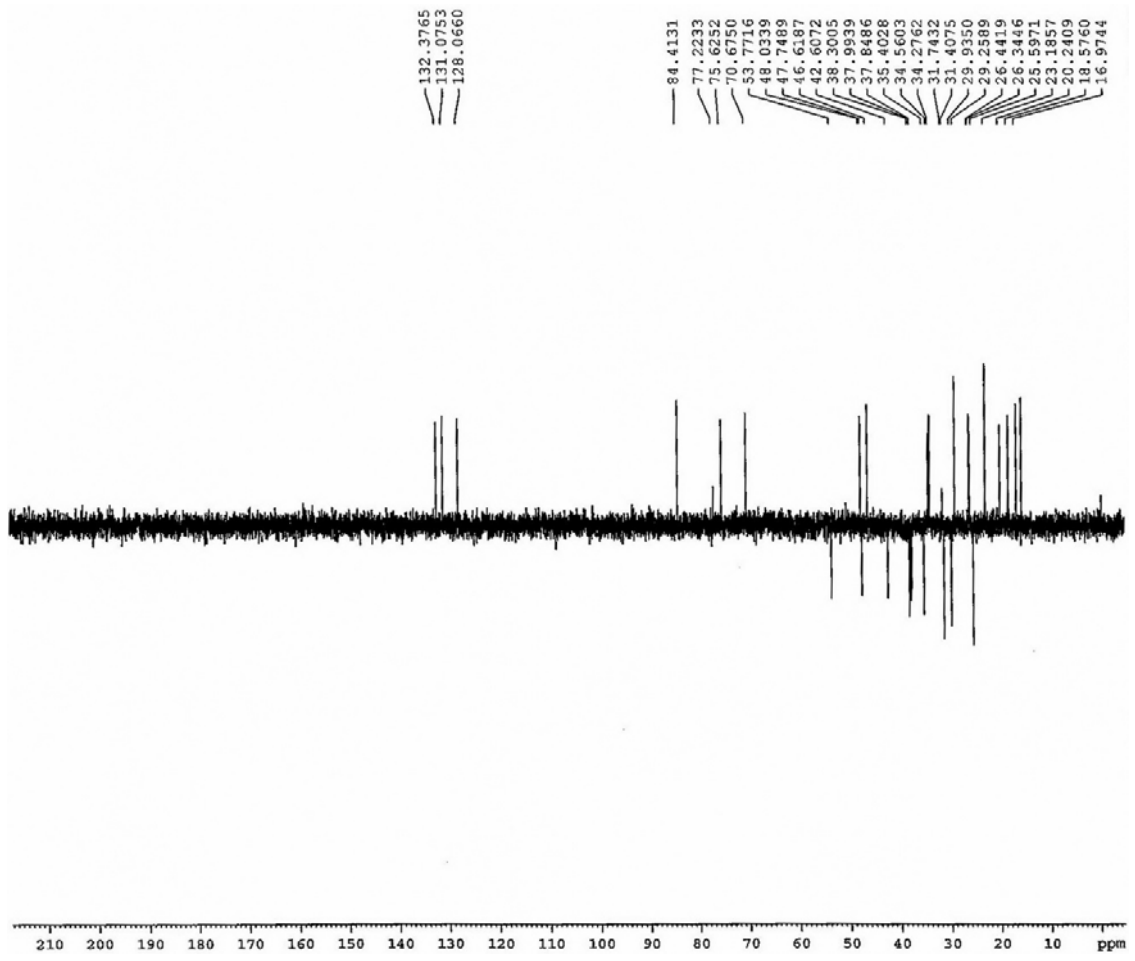
Page 1: ¹H NMR spectrum of N-Acetylborrelidin B



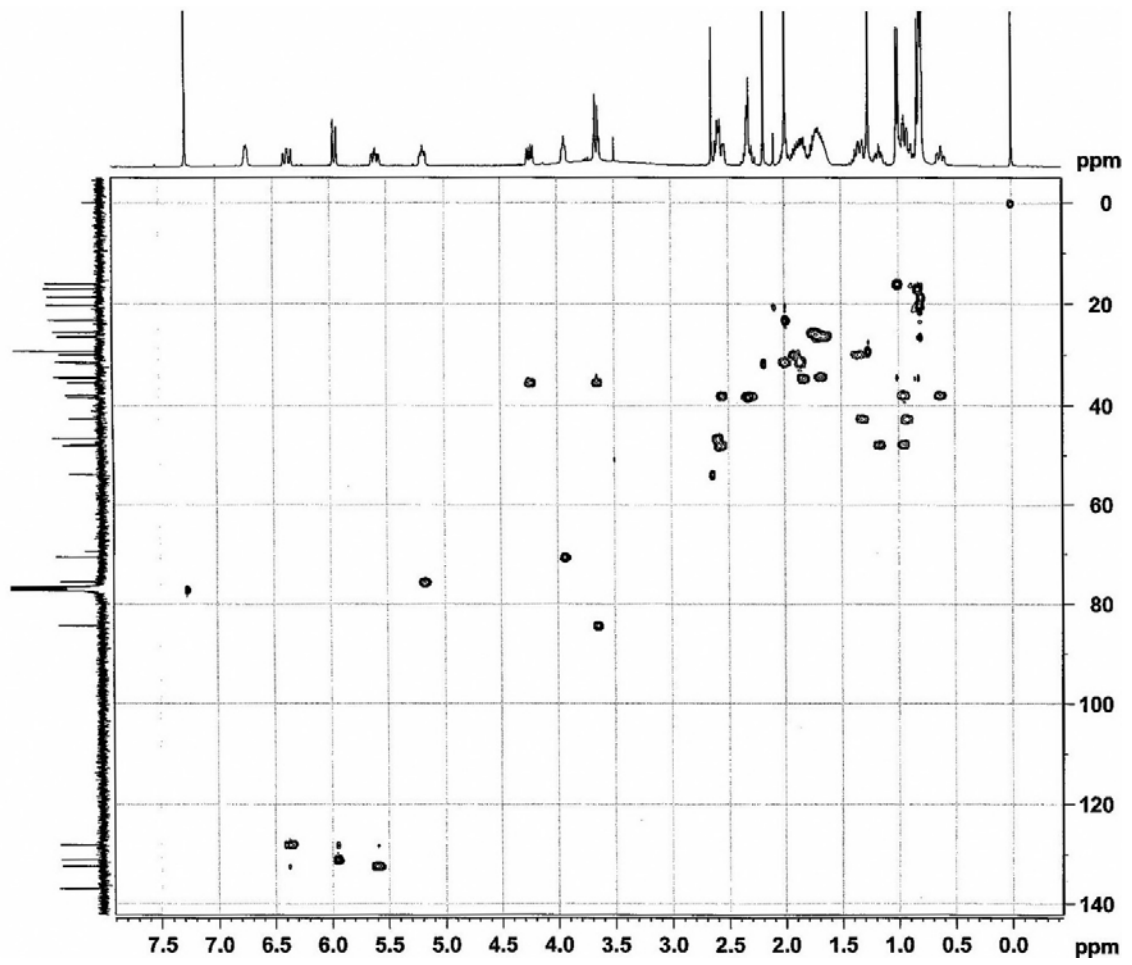
Page 2: ^{13}C NMR spectrum of N-Acetylborrelidin B



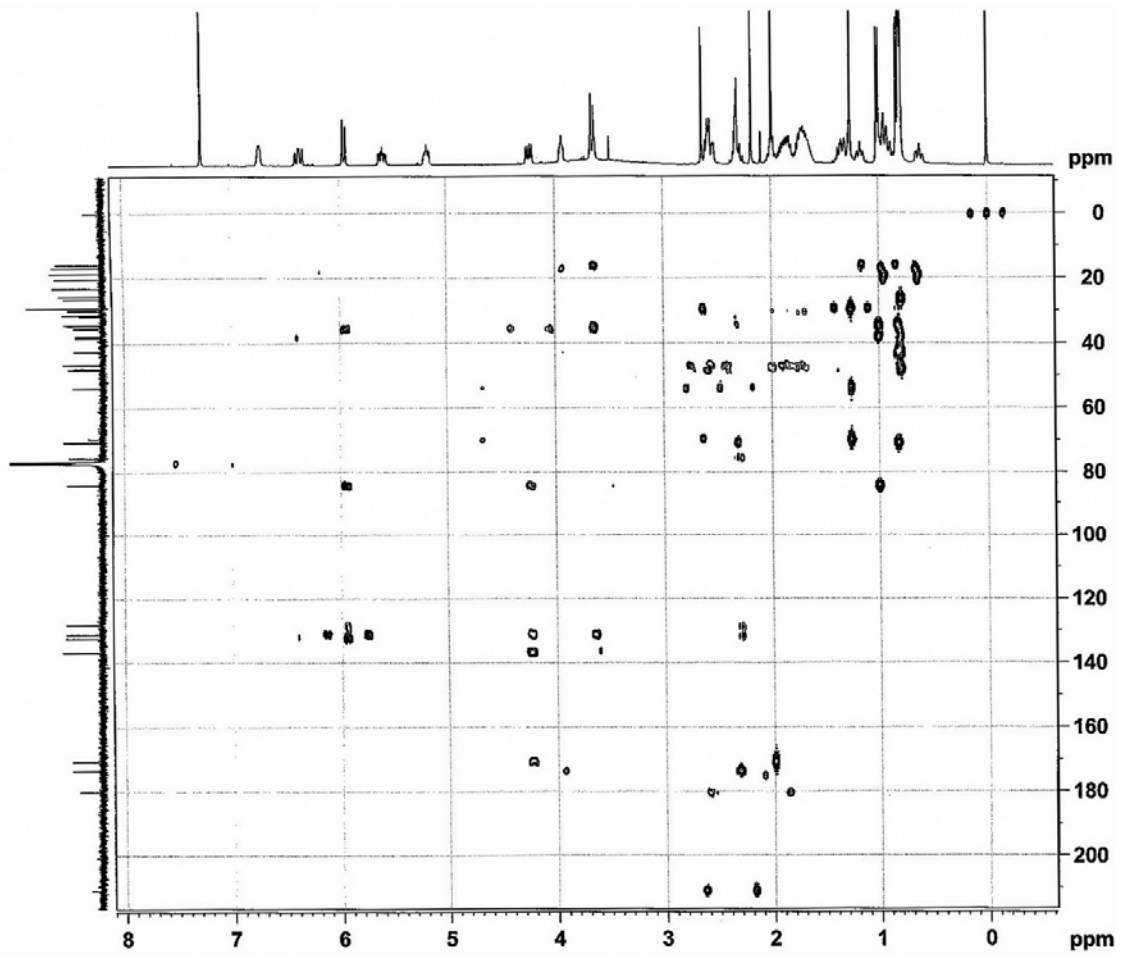
Page 3: DEPT 135 spectrum of N-Acetylborrelidin B



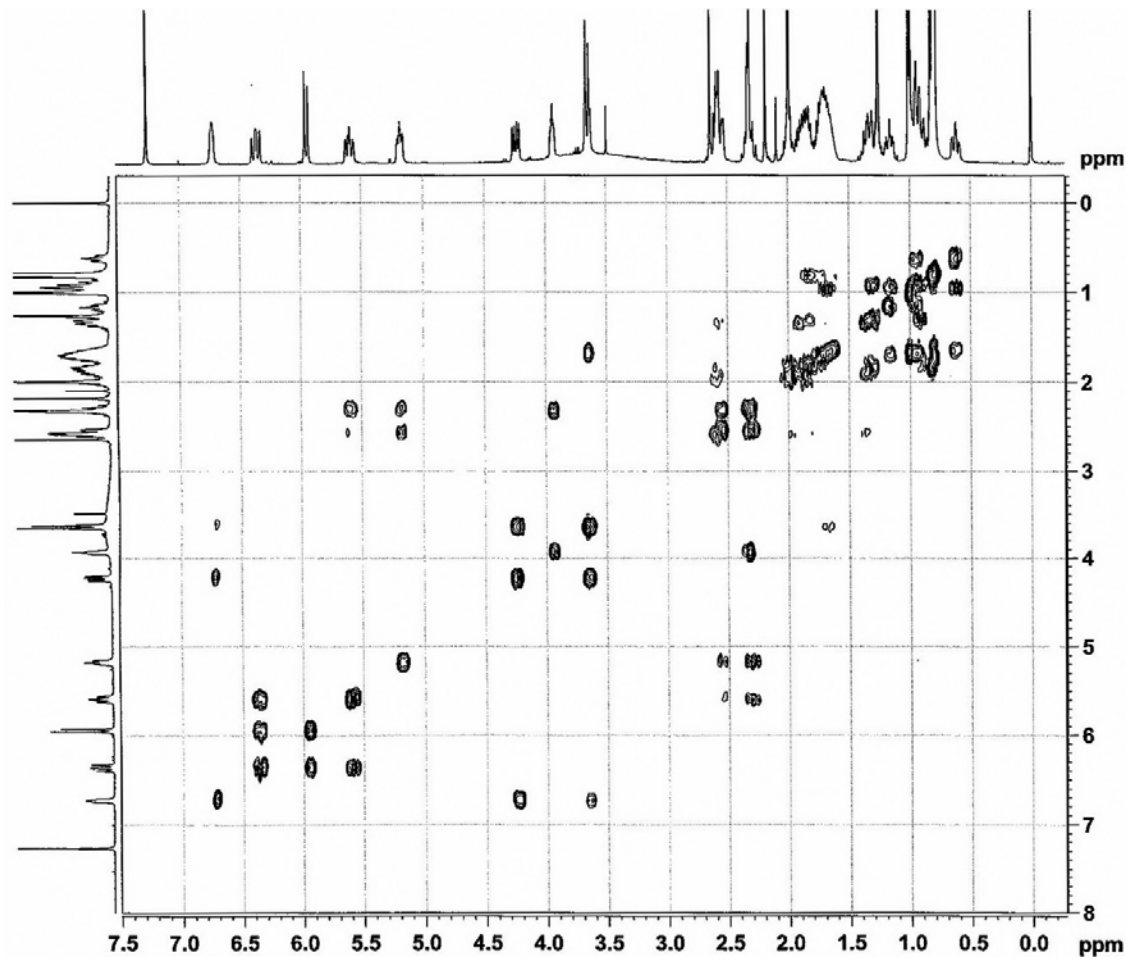
Page 4: HMQC spectrum of N-Acetylborrelidin B



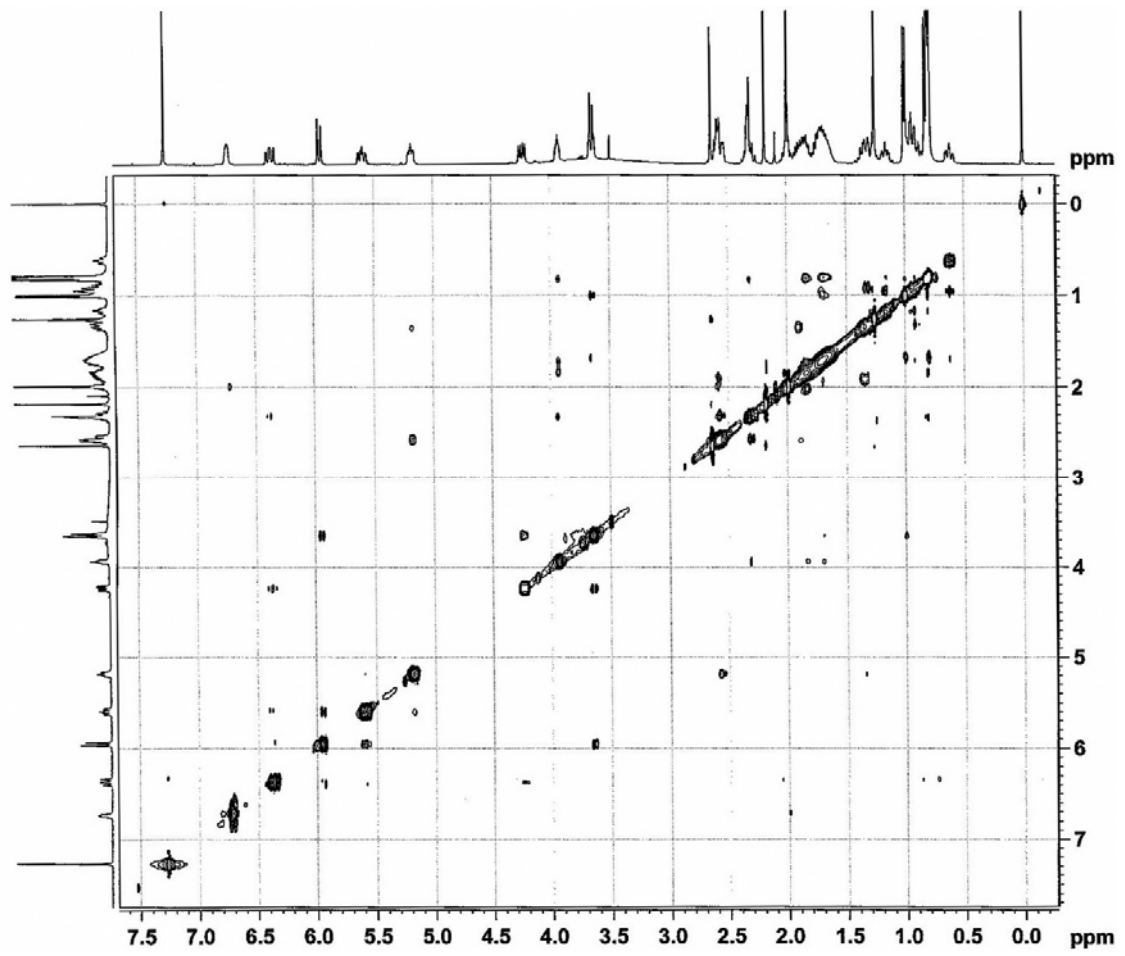
Page 5: HMBC spectrum of N-Acetylborrelidin B



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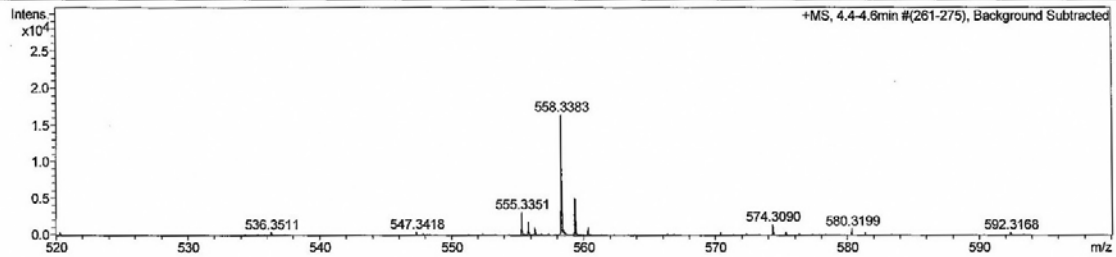
Page 7: NOESY spectrum of N-Acetylborrelidin B



Page 8: HR-MS spectrum of N-Acetylborrelidin B

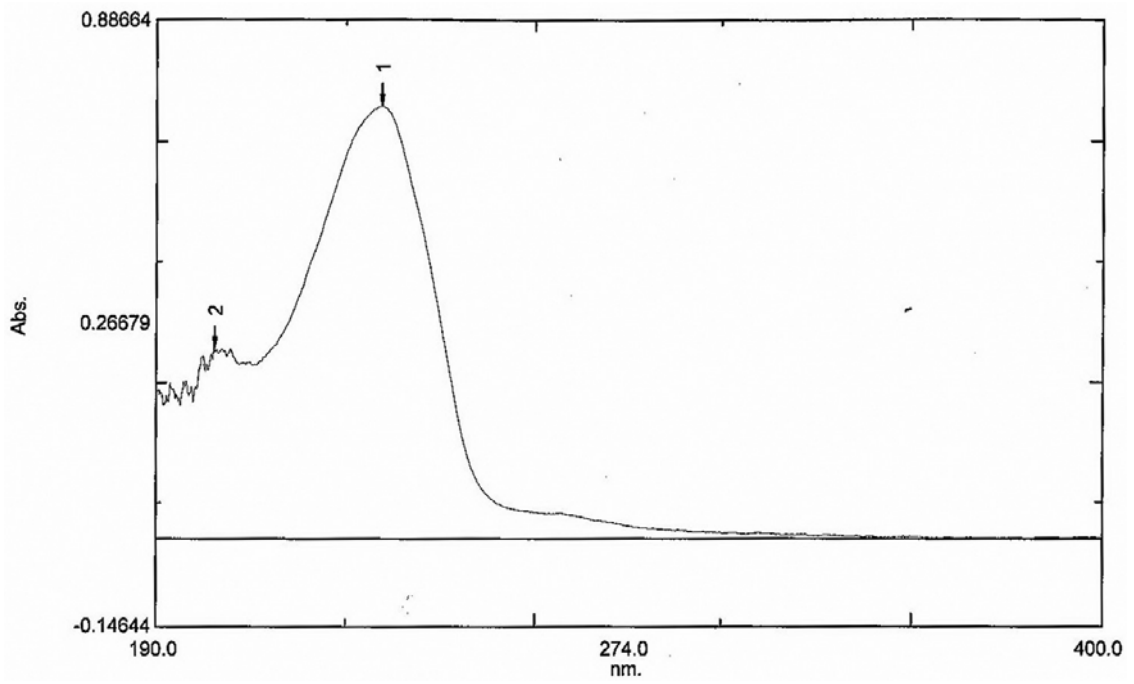
Acquisition Parameter

| | | | | | |
|-------------|----------|-----------------------|-----------|------------------|-----------|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 0.4 Bar |
| Focus | Active | Set Capillary | 4500 V | Set Dry Heater | 180 °C |
| Scan Begin | 50 m/z | Set End Plate Offset | -500 V | Set Dry Gas | 4.0 l/min |
| Scan End | 1000 m/z | Set Collision Cell RF | 120.0 Vpp | Set Divert Valve | Waste |

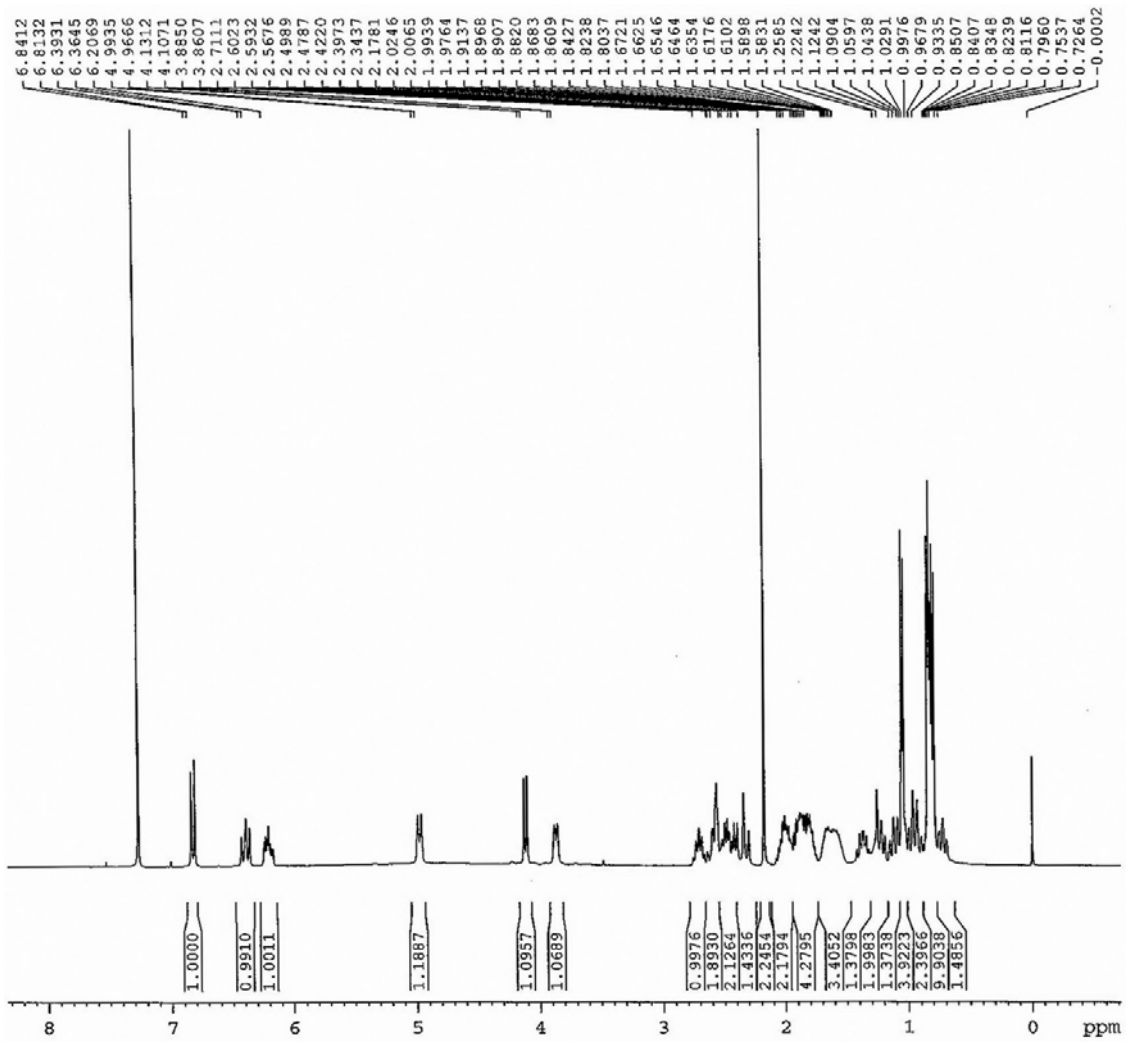


| Meas. m/z | # | Formula | m/z | err [ppm] | Mean err [ppm] | rdB | N-Rule | e ⁻ Conf | mSigma | Std I | Std Mean m/z | Std VarNorm | Std m/z Diff | Std Comb Dev |
|-----------|---|---|----------|-----------|----------------|------|--------|---------------------|--------|--------|--------------|-------------|--------------|--------------|
| 558.3383 | 1 | C ₂₅ H ₄₉ N ₃ NaO ₉ | 558.3361 | -3.9 | -3.6 | 2.5 | ok | even | 11.13 | 0.0199 | 0.0022 | 0.0064 | 0.0012 | 0.8345 |
| | 2 | C ₃₀ H ₄₉ N ₃ NaO ₇ | 558.3401 | 3.3 | 3.7 | 6.5 | ok | even | 12.99 | 0.0208 | 0.0023 | 0.0065 | 0.0012 | 0.8427 |
| | 3 | C ₃₇ H ₄₅ N ₃ NaO ₂ | 558.3343 | -7.2 | -6.8 | 15.5 | ok | even | 51.60 | 0.0780 | 0.0040 | 0.0243 | 0.0012 | 0.9781 |

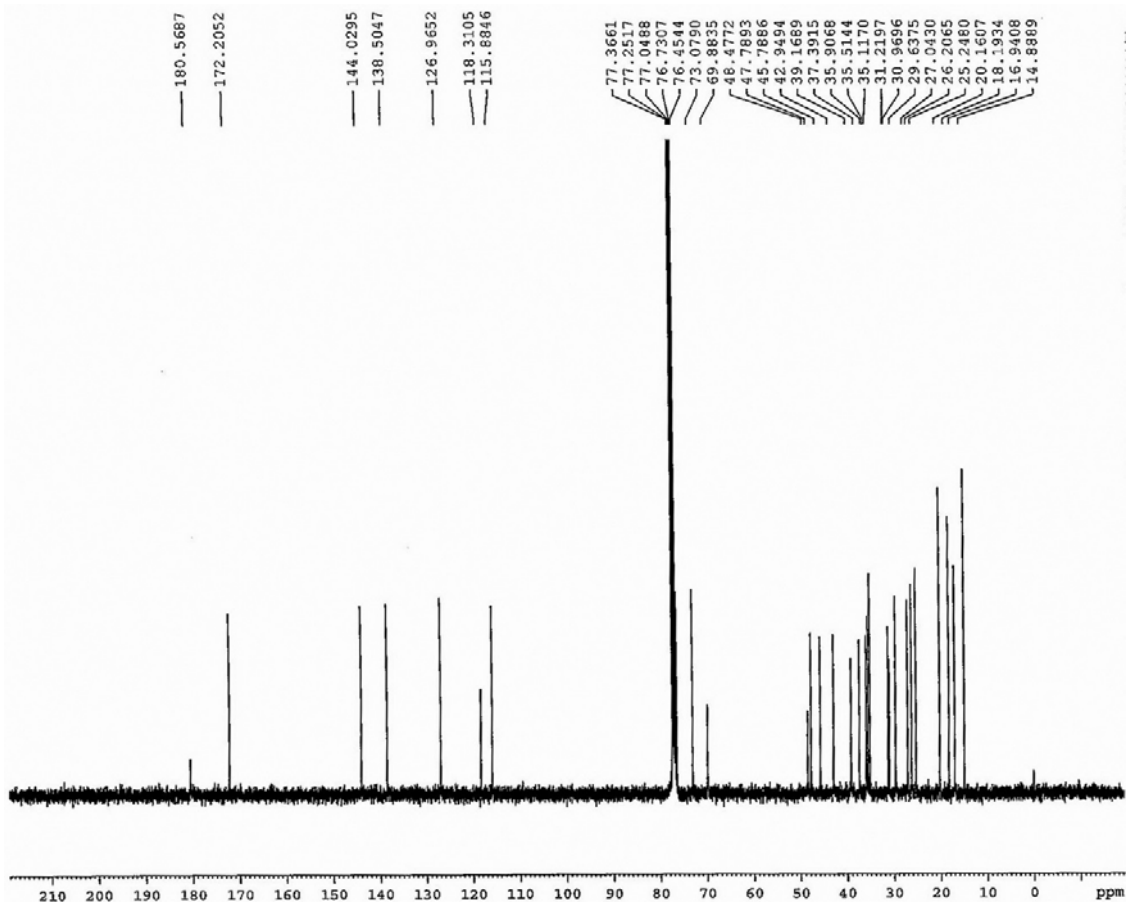
Page 9: UV spectrum of N-Acetylborrelidin B



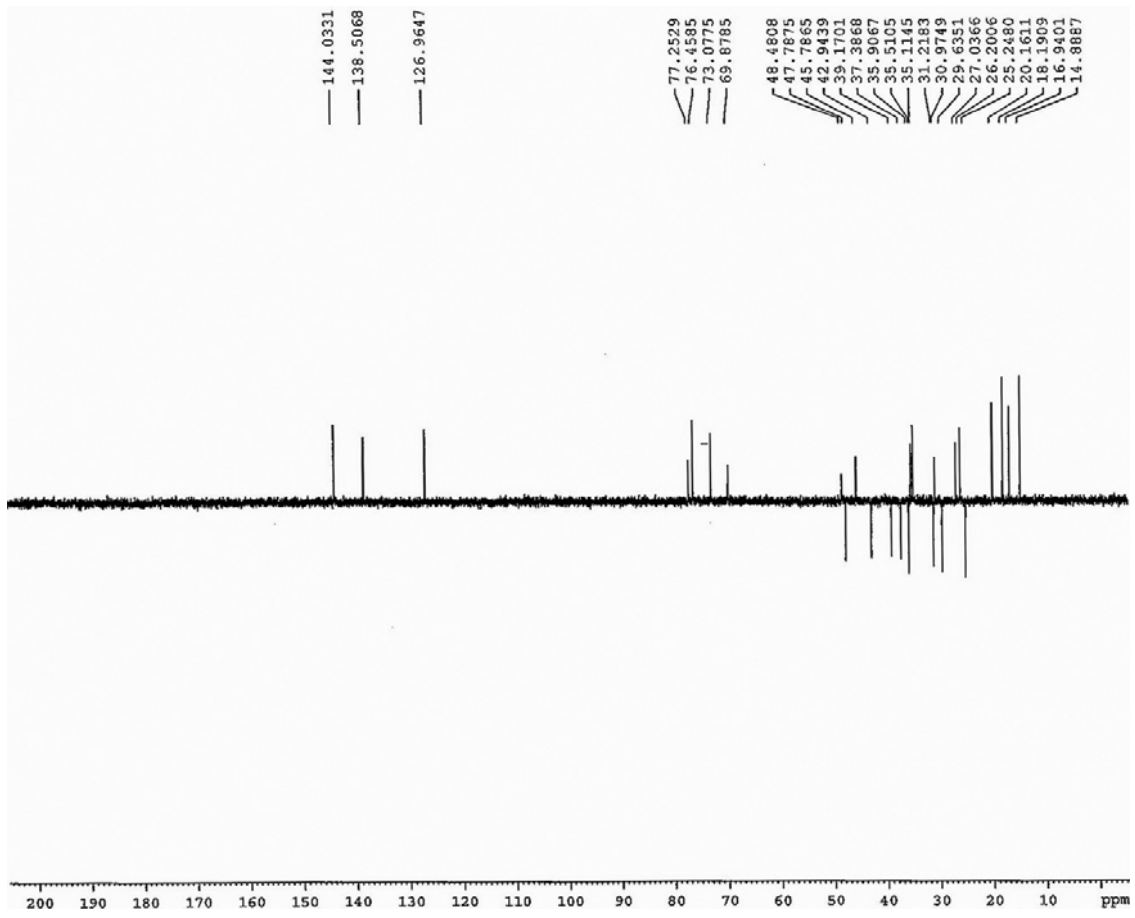
Page 10: ¹H NMR spectrum of borrelidin



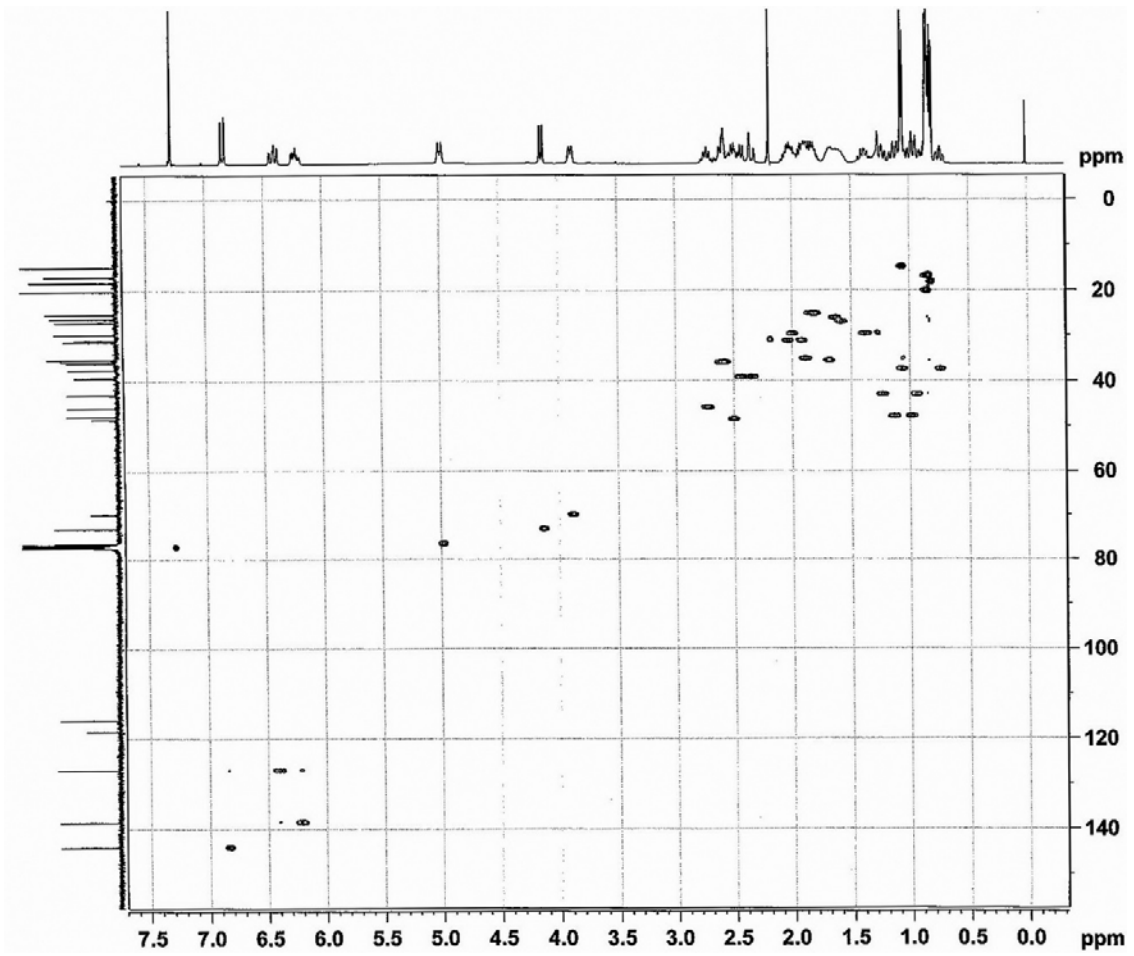
Page 11: ^{13}C NMR spectrum of borrelidin



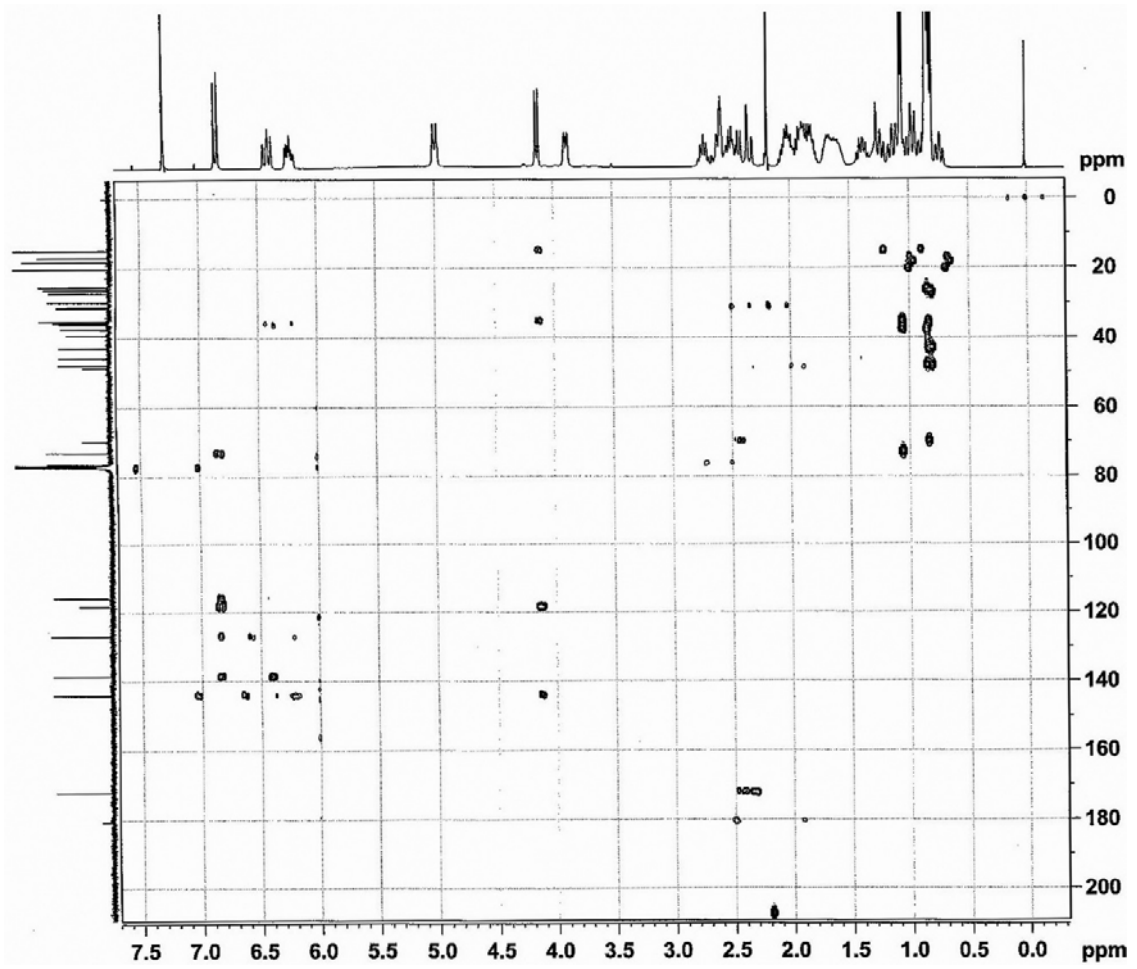
Page 12: DEPT135 spectrum of borrelidin



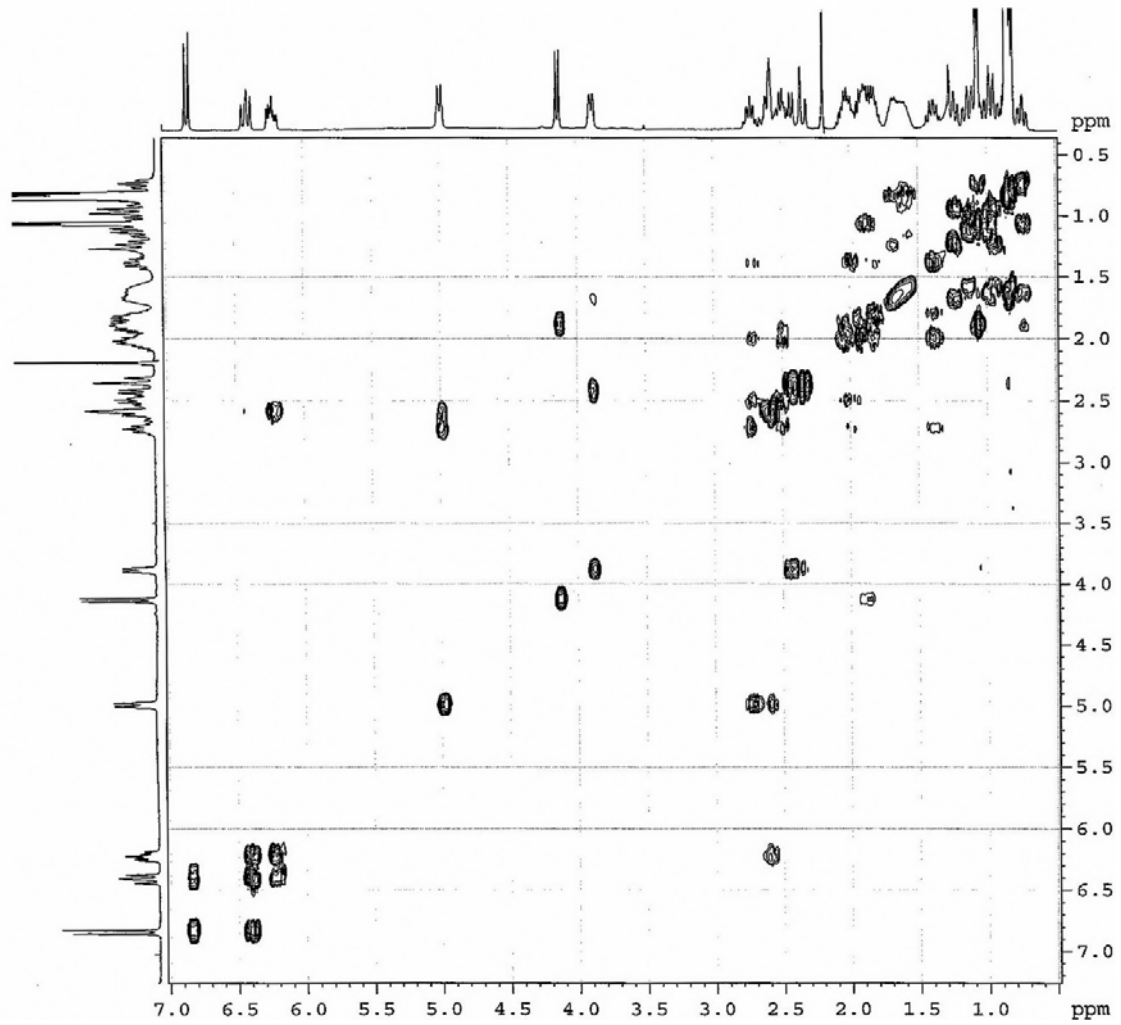
Page 13: HMQC spectrum of borrelidin



Page 14: HMBC spectrum of borrelidin



Page 15: COSY spectrum of borrelidin



Page 16: ESI-MS spectrum of borrelidin

F: - c ESI Full ms [300.00-700.00]

